



Opacity Calculations for Stellar Astrophysics

Jean-Christophe Pain^{1,2}

¹CEA, DAM, DIF, F-91297 Arpajon, France ²Université Paris-Saclay, CEA, Laboratoire Matière en Conditions Extrêmes, F-91680 Bruyères-le-Châtel Cedex, France



This work discusses results obtained through numerous collaborations, in particular with:

J. E. Bailey (SNL) S. Bastiani (LULI) C. Blancard (CEA) J. Colgan (LANL) Ph. Cossé (CEA) M. Dozières (General Atomics) G. Faussurier (CEA) F. Gilleron (CEA) D. Gilles (CEA) S. B. Hansen (SNL) R. M. More (Pleasanton, CA, USA) T. Nagayama (SNL) S. N. Nahar (Ohio State University) A. K. Pradhan (Ohio State University) F. Thais (CEA) S. Turck-Chièze (CEA)

Outline of the talk

- 1. Opacities and stars
- 2. Computation of opacity: the SCO-RCG code
- 3. Opacity comparisons in conditions representative of stellar envelopes
- 4. Spectroscopy experiments
- 5. Boundary of the convective zone of the Sun: the enigmatic Z-pinch experiment on iron

Part 1

Opacities and stars

■ In 1926, Eddington identifies opacity as a key parameter of stellar models.

■ In 1929, **Russell** publishes the first quantitative analysis of the chemical composition of the solar atmosphere, first made by **Payne-Gaposchkin** in 1924.

At such temperatures and densities, most of the elements are not fully ionized.

■ In the early sixties, **Cox** and **Huebner** introduce photo-excitation and photo-ionization processes in the calculation of stellar opacities.

Simon raises in 1982 the problem of the pulsation of Cepheids: opacity of « heavy » elements: C, N, O, ...

IS THE METAL CONTRIBUTION TO THE ASTROPHYSICAL OPACITY INCORRECT? N. H. MAGEE, JR., A. L. MERTS, AND W. F. HUEBNER T-4, Los Alamos National Laboratory Received 1983 November 22: accepted 1984 February 15 ABSTRACT Numerical tests by Simon have indicated that an arbitrary increase in the metal (atomic number Z > 2) contribution to the opacity by a factor of 2 to 3 leads to Cepheid models that, in some aspects, are in better agreement with observations than models using the standard opacity. We show that such a large increase in opacity is incompatible with atomic physics. Subject headings: atomic processes — opacities — stars: Cepheids — stars: interiors — stars: pulsation

1990's: OPAL (LLNL) and OP (Opacity Project = international academic collaboration): first stellar opacity tables.

N. H. Magee, Jr., A. L. Merts & W. F. Huebner, Astrophys. J. 283, 264 (1984).

Hydrostatic equilibrium:

Mass:

$$\begin{aligned}
\frac{dP}{dr} &= -\frac{Gm\rho}{r^2} \\
\frac{dm}{dr} &= 4\pi\rho r^2
\end{aligned}$$
Luminosity:

$$\begin{aligned}
\frac{dm}{dr} &= 4\pi\rho r^2 \\
L &= -\frac{4\pi r^2 ac dT^4}{3\kappa_R \rho dr} \\
\frac{dL}{dr} &= 4\pi\rho r^2\epsilon
\end{aligned}$$
P: pressure
T: temperature
p: density
M: mass
L: luminosity
s: energy
r: radius
a: Stefan's constant
c: speed of light
\end{aligned}

Rosseland mean
opacity

Part 2

Opacity calculation

The SCO-RCG code

Processes contributing to radiative opacity for local-thermodynamic-equilibrium plasmas

Opacity
Characterizes the interaction between electromagnetic radiation and matter by
absorption and scattering processes at a frequency v

$$K_{v}(\rho,T) = \frac{N_{\text{Avo}}}{A} \sum_{i} \bigoplus_{i} (\rho,T) \left\{ \sigma_{i,v}^{(\text{abs})}(\rho,T) \times [1 - \exp(-hv/k_{\text{B}}T)] + \sigma_{i,v}^{(\text{scat})}(\rho,T) \right\}$$
Occupation probability

$$X^i_a(E_a) + \hbar\omega \to X^i_b(E_b)$$

Photo-ionization (edges):

$$X_a^i(E_a) + \hbar\omega \to X_b^{i-1}(E_b) + \epsilon_b \qquad ; \qquad \hbar\omega = E_b + \epsilon_b - E_a$$

Inverse Bremsstrahlung:

$$\begin{split} X^i_a(E_a) + \epsilon_a + \hbar \omega &\to X^i_b(E_b) + \epsilon_b \quad ; \\ \hbar \omega &= E_b + \epsilon_b - (E_a + \epsilon_a) \end{split}$$



Scattering of a photon by free electrons (Compton) and by bound electrons (Rayleigh).



¹F. J. D. Serduke, E. Minguez, S. J. Davidson and C.A. Iglesias, JQSRT 65, 527 (2000).

The SCO-RCG code¹: opacity of local-thermodynamic-equilibrium (LTE) plasmas



Strengths : completeness (large number of excited states) and density effects on the wavefunctions.

Weakness: configuration interaction only inside non-relativistic configurations.

¹J.-C Pain and F. Gilleron, High Energy Density Phys. 15, 30 (2015).
²T. Blenski, A. Grimaldi & F. Perrot, J. Quant. Spectrosc. Radiat. Transfer 65, 91 (2000).
³J.-C Pain, G. Dejonghe and T. Blenski, J. Quant. Spectrosc. Radiat. Transfer 99, 451 (2006).
⁴R. D. Cowan, The Theory of Atomic Structure and Spectra, 1981.

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Part 3

Comparisons of opacities in conditions representative of stellar envelopes



Computed pattern of a p-mode solar acoustic oscillation of the Sun (l=20, m=16, and n=14.) © CC

Envelopes of β Cephei-type stars

I In 1902, Edwin Frost discovers the variability of the radial velocity of β Cephei (β Canis Majoris).

- β Cephei type stars (8 to 18 M_{\odot}):
- Hot blue-white stars of spectral class B.
- Ex: v Eridani, γ Pegasi, β Crucis, β Centauri...
- Opacity of the « iron group » (Cr, Fe & Ni):
- T \approx 200-300,000 K and $\rho \approx 10^{-7} \text{--} 10^{-6} \, g/cm^3$
- The iron-group opacity peak excites acoustic (p) modes through the "kappa-mechanism".

• « Slowly Pulsating B » (SPB) stars are subject to gravity modes (« g » modes), also connected to iron opacity. Their mass is from 2 to 6 M_{\odot} .

E. B. Frost, "The Period of Beta Cephei", Astrophys. J., 24, 259 (1906).

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β Cephei (Alfirk) (© Palomar Observatory)

Magnitude: +3.16 to +3.27. Period: 4.57 hours. Fe, T=23 eV, ρ =2 mg/cc

• Stellar envelopes of β Cephei type stars: $\rho \approx 10^{-6}$ g/cm³ and T ≈ 30 eV.

Equivalent conditions of mean ionization with higher density accessible to experiment.



Fe, T=23 eV, ρ =2 mg/cm³

Fe Rosseland mean opacities

ATOMIC « full »	ATOMIC n5	SCO-RCG
19508	15205	18510

ATOMIC code (OPLIB tables)¹ (Los Alamos National Laboratory)

"n5": limited to n_{max}=5 but includes configuration interaction. "full": large number of states but no configuration interaction.

120

SCO-RCG ATOMIC n5

100

Dilemna: completeness or accuracy?

¹J. Colgan et al., ApJ **817**, 116 (2016). S. Turck-Chièze et al., ApJ **823**, 78 (2016).

T (eV)	n _e (cm⁻³)	ρ (g/cm³)	OP (cm²/g)	ATOMIC « full » (cm²/g)	SCO-RCG (cm²/g)
10.8	1017	1.35 10 ⁻⁶	24.7	64	62.6
15.3	3.16 1017	3.44 10 ⁻⁶	358	682.3	673.8
17.2	1017	9.52 10 ⁻⁷	354	486,2	499.2
21.6	1018	8.85 10 ⁻⁶	1270	1359	1313
25.5	3.16 1017	2.44 10 ⁻⁶	232	130.6	121.9

S. Turck-Chièze et al., ApJ 823, 78 (2016).



(*) - This group of lines, in the center: radium, isnt'it?... - Radium? No way! ...



Principle of a laser spectroscopy absorption experiment









S. J. Davidson et al., App. Phys. Lett. 52, 847(1988).



C. Chenais-Popovics, Laser Part. Beams **20**, 291 (2002). M. Sako et al., A&A **365**, L368 (2001).



G. Xiong et al., Astrophys. J. 816, 36 (2016).Silicates: - around AGB stars and in disks around Ae/Be stars.J.-C. Pain, F. Gilleron and M. Comet, Atoms 5, 22 (2017).- processed in the diffuse interstellar medium.





M. Dozières et al., High Energy Density Phys. 17, 231 (2015).





C SNL

Figure: Experimental setup (©Sandia National Laboratory).

- (a) The two concentric tungsten cages and the central plastic foam (CH_2) .
- (b) When the tungsten plasma collides with the CH₂ foam, the shock-generated radiation is trapped in the tungsten cages and heats the sample.
- (c) At stagnation, an intense radiation (backlighter) is created, used to probe the sample (radiography).



J. E. Bailey et al., Phys. Rev. Lett. 99, 265002 (2007).

Part 5

Base of the solar convective zone

The enigmatic iron experiment



© EIT/SOHO Fe IX 171 Å, *T*=7 10⁵ K ; Fe XII 195 Å, *T*=1.4 10⁶ K ; Fe XV 284 Å, *T*=2 10⁶ K

Iron opacity at different distances from the Sun center

		\mathbf{m}^{3} R/	R
1345.7	78 152.0)55 ()
340.70	01 1.297	'18 O.	5
188.1	.8 0.188	062 0.7	13
	Fe Z*=15 T=188 ρ=1,13	.088 .18 eV 8 g/cc	
	Ion charge 13	Fraction 0.0188	
	14	0.127	
	16	0.338	
	17	0.180	
	18	0.0421	
	19	0.00385	
	20	0.000132	

■ Iron contributes for 25 % of the total opacity at the BCZ (boundary of the convective zone) of the Sun.



From the radiative zone to the convective zone: the BCZ

Recent reevaluation of the abundances of C, N and O in the solar mixture enhanced the disagreement between heliosismic measurements and predictions of the SSM (Standard Solar Model).

In order to reconcile observations and modeling, a 5 to 20 % increase would be necessary.

Fe, T=192 eV, n_e=3.1 10²³ cm⁻³



Analysis of 3D convective atmospheres

Element	Previous	New
	abundances ¹	abundances ²
Н	12	12
Не	10,93	10,93
С	8,52	8,43
Ν	7,92	7,83
0	8,83	8,69
Fe	7,50	7,50

<u>Table:</u> $A_x = Log_{10}(N_x/N_H) + 12$, where N_x is the number of atoms of element X (H, He, C, N, O et Fe).

¹N. Grevesse & A. J. Sauval, Space Sci. Rev. **85**, 161 (1998). ²M. Asplund and N. Grevesse, A. J. Sauval & P. Scott, A&A **47**, 481 (2009).

J. Colgan et al., ApJ **817**, 116 (2016).

■ Purpose: measuring iron transmission in conditions close to the ones of the BCZ.



<u>Figure</u>: Iron opacity at T \approx 2.11 MK and n_e= 3.1x10²² e-/cm³. The experimental spectrum (black) is compared to three calculations: ATOMIC (USA), SCO-RCG and OPAS (CEA, France).

• Inclusion the measured spectrum in a Rosseland average for a solar mixture \rightarrow 7 % increase.

J. E. Bailey et al., Nature **517**, 56 (2015).

Courtesy G. Loisel, J. E. Bailey, T. Nagayama, S. B. Hansen





J.-C. Pain and F. Gilleron, High Energy Density Phys. 15, 30 (2015).



Fe SCO-RCG conditions: T=182 eV ρ =0.17 g.cm⁻³ (n_e=3.1 10²² cm⁻³)

C. T. Chantler, J. Phys. Chem. Ref. Data 24, 71 (1995).
B. L. Henke et al., At. Data Nucl. Data Tables 54, 181 (1993).
C. A. Iglesias, High Energy Density Phys. 15, 4 (2015).

Nahar and Pradhan reported extensive R-matrix calculations of unprecedented complexity for ion Fe XVII and found large enhancement in photo-ionization cross-sections, in addition to strongly peaked photo-excitation-of-core resonances.



S. N. Nahar et al., Phys. Rev. A **83**, 053417 (2011). [60 LS core states]. <u>http://cdsweb.u-strasbg.fr/topbase/topbase.html</u> S. N. Nahar and A. K. Pradhan, Phys. Rev. Lett. **116**, 235003 (2016). [99 LS core states].

- C. Blancard et al., Phys. Rev. Lett. 117, 249501 (2016).
- S. N. Nahar and A. K. Pradhan, Phys. Rev. Lett. 117, 249502 (2016).

■ We are performing calculations to figure out whether there is a strong two-photon opacity effect.



The mystery arises in a context of uncertainty in modeling the Solar interior.

Quantum theory of two-photon emission/absorption published by Goeppert-Mayer¹ in 1931 and applied to emission from metastable hydrogen in interstellar space by Breit and Teller².

Two-photon cross-sections are obtained using Fermi's "Golden Rules" for quantum perturbation theory.

¹M. Goeppert-Mayer, Ann Phys 9, 273 (1931). ²G. Breit and E. Teller, ApJ **91**, 215 (1940).

- > One should consider two photons of different energies $\hbar\omega_1$, $\hbar\omega_2 \rightarrow \sigma(\omega_1, \omega_2)$.
- $\omega_1 = \omega_2$ occurs only by accident and makes a tiny contribution.
- > I made a one-color calculation² and found $\sigma(\omega_1, \omega_1)$ was too small... So did M. Kruse ans C. Iglesias³...

Everybody agree it's too small, but it's not the right process!

> Photon ω_1 is from the backlighter, the other photon is from the plasma or from the backlighter. Total photon energy is constrained : $\hbar\omega_1 + \hbar\omega_2 = \Delta E = E_{\text{final}} - E_{\text{initial}}$.

- > For any $\hbar\omega_1 (< \Delta E)$, there can be a second photon that has the right energy $\hbar\omega_2 = \Delta E \hbar\omega_1$.
- It is a continuous absorption, even for bound-bound transitions.
- It should be compared to the low-opacity gaps between one-photon lines.

The integral is much larger than the cross-section for two identical photons.

¹R. M. More, S. B. Hansen and T. Nagayama, High Energy Density Phys. 24, 44 (2017).
²J.-C. Pain, High Energy Density Phys. 26, 23 (2018).
³M. Kruse and C. Iglesias, High Energy Density Phys. 31, 38 (2019).
⁴R. M. More, J.-C. Pain, S. B. Hansen, T. Nagayama and J. Bailey, High Energy Density Phys., in press (2019).

Two-photon perturbation theory (collaboration R. M. More)



Kruse-Iglesias calculations include two-photon ionization cross-sections for ground as well as singly and doubly excited configurations of different charge states of Fe. Similar calculations were done for Cr and Ni.

Conclusions of the authors:

(i) All the two-photon ionization cross-sections were found to be more than 3 orders magnitude smaller than the corresponding single-photon one¹.

(ii) The ratio of two- to one-photon ionization cross-sections displays a weak dependence on nuclear charge along an isoelectronic sequence.

(iii) Furthermore, earlier work² showed two-photon ionization increasing with decreasing temperature. Such behavior cannot the discrepancies between experimental and theoretical results at the higher energies only for Fe at high temperature (Anchor 2).

■ Work is in progress to include more ions / states in the calculation³.

¹M.K.G. Kruse & C.A. Iglesias , HEDP **41**, 100976 (2021). ²M.K.G. Kruse & C.A. Iglesias, HEDP **31**, 38 (2019). ³R. M. More, J. E. Bailey and J.-C. Pain, work in progress. Photon scattering is also a two-photon process.

It is often included in opacity models assuming the Thomson cross-section.

As in two-photon absorption, however, scattering displays resonances whenever one of the photon energies coincides with the energy differences between bound states involved. That is, the resonances occur at the same photon energies as single photon spectral lines.

Kruse-Iglesias: Away from the resonances, Rayleigh (elastic) and Raman (inelastic) scattering are comparable or smaller than the Thomson scattering cross-section¹, and thus unlikely to contribute much.

Resonant inelastic X-ray scattering (RIXS), which can be described as a Raman effect, was observed in recent experiments on the large free-electron X-ray laser LCLS. As Compton scattering reduces x-ray transmission, so does the RIXS scattering.
Work is in progress to quantify its impact².

Baggott, Rose and Mangles suggest an additional process in which a non-resonant photon is absorbed and the intermediate state is stabilized by an electron collision³.

¹K. McNamara, D.V. Fursa & I. Bray, Phys. Rev. A **98**, 043435(2018).
²R. M. More, J. E. Bailey and J.-C. Pain, work in progress.
³R. A. Baggott , S. J. Rose and S. P. D. Mangles, Phys. Rev. Lett. **125**, 145002 (2020).

Transient localization effect

■ Liu et al. developed a formalism to study the wavefunctions of the continuum electrons that takes into account the quantum de-coherence caused by coupling with the plasma environment¹.

They find that the photoionization cross section of Fe¹⁶⁺ is considerably enhanced, which partly explains the big difference between the measured opacity and the models.

Novelty to account for plasma effects = replacement of the final continuum energy eigenstate with a wave packet, which energy is conserved in the photon ionization.

Iglesias' criticisms:

(i) First, the wave packet is assumed a stationary state (to apply the Golden Rule) even though it does not have a specific energy eigenvalue.

(ii) A second *ansatz* for the wave packet density of states ensures the formulas reduce to the distorted wave result in the absence of the plasma.

(iii) Finally, the velocity form of the photon-electron interaction is replaced with an approximate length form = reasonable for the Sandia experiments but may fail for more strongly coupled plasmas or high photon energies².

¹P. Liu, C. Gao, Y. Hou, J. Zeng, *et al.*, Commun. Phys., 95 1 (2018) ²C. A. Iglesias, HEDP **47**, 101043 (2023).

Convection Zone Base: T_e =185 eV, n_e = 90e21 e/cc

Data at T_e =156 eV, n_e = 7e21 e/cc Calculated opacity*



Data at T_e =182 eV, n_e = 38e21 e/cc Calculated opacity





Courtesy G. Loisel, J. E. Bailey, T. Nagayama, S. B. Hansen



- T_e and n_e are diagnosed independently
- Reproducibility is confirmed



Why is two-photon absorption significant for Fe but not for Ni?

■ Since the energies are ~200 eV larger for Ni than for Fe, the cross-section and the population from the Bose-Einstein factor are smaller. The 2-photon process in Ni is 10 times smaller than for Fe. That helps to understand why it is not visible in the experiments. At a higher temperature, it might be visible.



Can we check accuracy of modeled line shapes?

Courtesy G. Loisel, J. E. Bailey, T. Nagayama, S. B. Hansen



We use $n=2 \rightarrow 4$ lines from Ne-like Ni to assess the accuracy of calculated line shape







Solar mixture @ T=188.18 eV & $n_e = 10^{23}$ cm⁻³

M. Asplund and N. Grevesse, A. J. Sauval & P. Scott, A&A 47, 481 (2009).

	к _Р (cm2/g)	к _R (cm2/g)
No ionic Stark	1685	273.5
With ionic Stark	1719	285.3



Magg et al. new abundances

New observational material for the Sun, new updated atomic data, and up-to-date NLTE models to re-analyse the detailed chemical composition of the solar photosphere.

Two families of **3D radiation-hydrodynamics simulations of solar convection**, to quantify the differences between the abundances inferred with both models.

New estimates of chemical abundances for C, N, O, Mg, Si, Ca, Fe, and Ni.

■ Solar photospheric Z/X ratio = 0.0225, when calculated using the photospheric abundances only, and 0.0226, when meteoritic abundances used for most species, except C, N, and O, for which the photospheric values are used.

■ Magg et al.'s estimates are 26% higher compared to those determined by Asplund et al. (2021), but in a much better agreement with Caffau et al. (2011) and Grevesse & Sauval (1998), the difference being 10% and 1%, respectively.

■ Very close numerical agreement of Z/X with Grevesse & Sauval (1998) is, however, fortuitous, as abundances of individual elements are different in their study.

Magg. et al., A&A 661, A140 (2022).

■ We are performing calculations to figure out whether there is a strong two-photon opacity effect.

■ To our knowledge, the problem of acceleration (diffusion) induced by two-photon radiation was never studied before. Astrophysicists usually take opacity tables (mostly OP and OPAL) as an input of their radiative-acceleration calculations.

■ A phenomenon might be affected: the so-called "saturation effect". When matter density increases, the number of ions per volume unit getting higher, the number of available photons likely to yield the acceleration decreases.

S. Turcotte, J. Richer, G. Michaud, C. A. Iglesias and F. J. Rogers , ApJ 504, 539 (1998).

G. Alecian and F. LeBlanc, MNRAS 319, 677 (2000).

G. Vauclair and S. Vauclair, « Competition between diffusion processes and hydrodynamical instabilities in stellar envelopes », *Edith A. Muller (ed.), Highlights of Astronomy, Vol.* 4, *Part II,* 193-203 (1977).

- Opacity computation requires to take into account a huge number of levels and spectral lines.
- Some effects, such as **configuration interaction**, are still difficult to take into account properly.
- Some laser or **Z-pinch** experiments are performed in order to test the models.
- The unexplained iron experiment on Z stimulates new developments in the codes (photo-ionization, highly-excited states, two-photon processes^{1,2}, etc.).
- In the same conditions, the Ni spectrum is in good agreement with SCO-RCG³.

■ An experiment is ongoing on NIF (National Ignition Facility) laser facility in order to measure iron opacity in the same conditions as the Z experiment.

¹R. M. More, S. B. Hansen and T. Nagayama, High Energy Density Phys. 24, 44 (2017).
²J.-C. Pain, High Energy Density Phys. 26, 23 (2018).
³J. E. Bailey et al., to be published.

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Important issues for improvement of opacity calculations

■ Need for detailed accurate and complete energy levels, line energies, *f*-values and cross-sections for atoms/ions/anions/molecules and transient ion dipoles formed in collisions¹.

■ The steady increase in computing power should ease the accuracy / completeness compromise.

Plasma density effects: pressure ionization (quasi-bound states), realistic microfield distributions for reliable line broadening.

Quantum-mechanical calculation of continuum absorption: bound-free and free-free.
 Continuity of oscillator strength must be ensured.

■ Proper accouting for plasma oscillations on the dielectric constant²: electron degeneracy and screening.

Continue helioseismological work.

¹A. E. Lynas-Gray et al. « Current State of Astrophysical Opacities: A White Paper », arXiv:1804.06804v1. ²B. M. Sarfraz et al., Phys. of Plasmas **25**, 032106 (2018).